The Scaling Properties of Atomistic Fluid Dynamics Simulations

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Fluid dynamics is usually described by continuum models such as the Navier-Stokes (NS) equation, and such models have had great success in describing real-world phenomena. In addition, the results can often be scaled in various ways to describe an entire class of related systems. However, the validity of continuum models is in practice an emergent phenomenon of the underlying dynamics of the atoms comprising the fluid. In recent years, the available computational capacity has increased to the point where direct simulation of these underlying atomistic dynamics has become possible for increasingly large systems [1]. Nevertheless, there has been considerable resistance to the acceptance of such simulations. In particular, it has been asserted that they do not scale, i.e., that the results of atomistic simulations at the largest scales currently accessible (~50 μm) are not relevant to the description of larger, macroscopic systems.

The Navier-Stokes equation with gravity,

$$\rho\left(\partial_t u + u \cdot \nabla u\right) = -\nabla p + \mu \Delta u + \rho g$$

is invariant under the transformation $u \rightarrow u/a$, $x \rightarrow ax$, $t \rightarrow a^2 t$, $g \rightarrow g/a^3$, $p \rightarrow p/a^2$. In order to determine if atomistic simulations possess a similar scaling, we have performed a series of direct simulation Monte Carlo (DSMC) simulations of the Rayleigh-Taylor instability (RTI), in which a heavy fluid initially lies on top of a light fluid in the presence of gravity. These simulations had various values of the gravitational acceleration g, and contained up to 5.7 billion particles. If these simulations obey the scaling described above, then expressing the dimensions of the system in terms of a scale length λ and a scale time τ, which scale with gravity as $\lambda \sim g^{-1/3}$ and $\tau \sim g^{-2/3}$, will cause the results of different-gravity runs to appear equivalent.

Figure 1 shows a series of snapshots in the development of the RTI for several gravities at various values of t/τ. Each image is ~50 λ in width. It is clear that these images are qualitatively similar for identical values of t/τ. To make this notion more quantitative, we have found that at $t/\tau = 14$ the fractal dimension D of the interface is — to within numerical uncertainty – the same for each of these gravities. Unscaled results for the bubble and spike positions as a function of time are shown in Fig. 2. Note that the length and time scales vary by factors of 5 and 26, respectively, between the lowest and highest gravities. Upon scaling by λ and τ, however, these results approximately collapse onto one another (Fig. 3). (The moderate disagreement for large t/τ can be attributed to the influence of the fluctuations and compressibility present in any atomistic simulation.) Furthermore, a scaled comparison between an atomistic simulation and experimental RTI results (Fig. 3, inset) shows similar agreement, even though the unscaled length and time scales differed by factors of 42×10^6 and 70×10^3, respectively, and the gravity differed by a factor of 10^{10}. This suggests that atomistic simulations can, in fact, be scaled up to describe macroscopic situations.

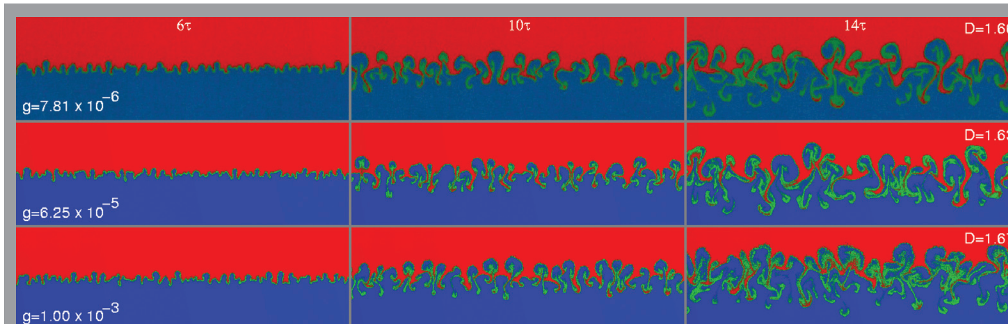

Fig. 1. Time evolution of the species field for different gravities and Atwood number A = 0.67 (red: heavy particles, blue: light particles, green: mixture). Snapshots at different times and gravities were chosen to show a subset of the system with a width of 50 λ. The fractal dimension D of the interface at $t/\tau = 14$ is given in the top right corner for each gravity. To within noise, the scaled results exhibit no difference for different gravities.

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[1] K. Kadau et al., *Proc. Nat. Acad. Sci*, **104,** 7741-7745 (2007).

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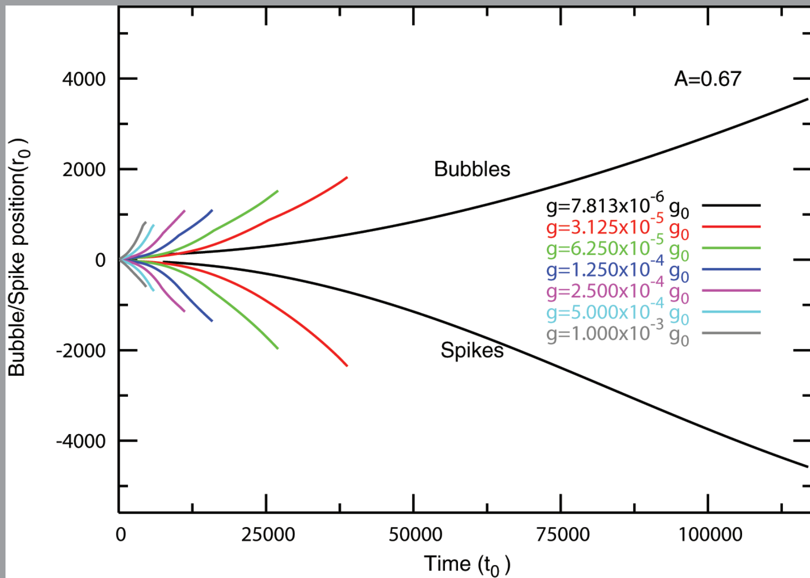

Fig. 2. Unscaled bubble and spike positions for different values of gravity and A = 0.67. The ratios between the largest and smallest length and time scale are 5 and 26, respectively.

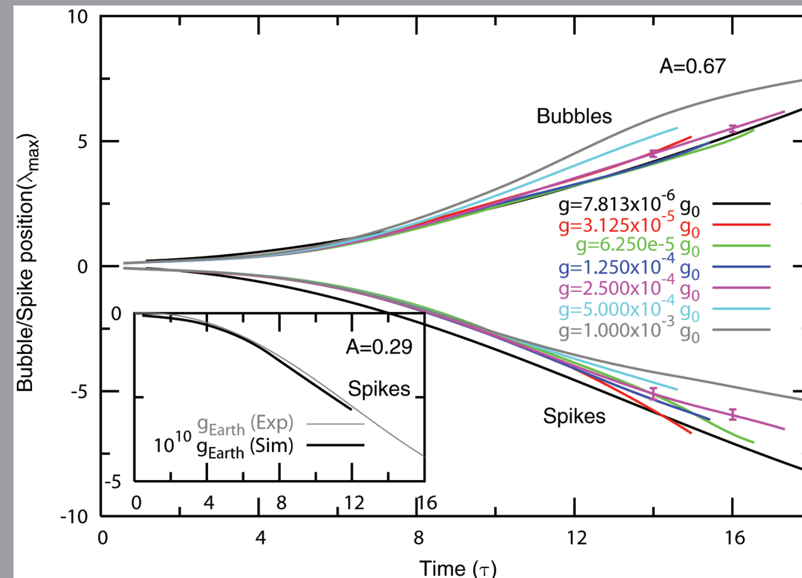

Fig. 3. Scaled bubble/spike positions for different values of gravity (same data as in Fig. 2). Inset: Scaled simulation and experimental spike positions, for which the unscaled length scales, time scales, and gravities differ by factors of 42 x 10^6, 70 x 10^3, and 10^{10}, respectively.